

Photoionization of Ne^+ : an absolute benchmark for theory

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The photoionization of ions is a fundamental process of importance in many high-temperature plasma environments, such as those occurring in stars and nebulae, as well as in inertial-confinement fusion experiments. Quantitative measurements of photoionization of ions provide precision data on ionic structure, and guidance to the development of theoretical models of multi-electron interactions. In addition, the opacity databases [1, 2] that are critical to the modeling and diagnostics of hot, dense plasmas consist almost entirely of untested coupled-state theoretical calculations based on the R-matrix method. High-resolution absolute photoionization cross-section measurements are therefore needed to benchmark these theoretical methods. Being the sixth-most abundant element in the universe, neon is significant in astrophysics, and therefore Ne^+ was selected for absolute measurements of photoionization cross sections to benchmark a state-of-the-art Breit-Pauli R-matrix theoretical calculation.

The experiments were performed on ALS beamline 10.0.1.2 using the ion-photon-beam (IPB) research endstation [3]. An energy-selected photon beam was merged over a path length of 29 cm with a highly collimated 6 keV Ne^+ beam produced in the hot-filament discharge ion source of the Cuernavaca ion gun apparatus. Two-dimensional intensity distributions of both beams were measured by rotating-wire beam profile monitors installed just upstream and downstream of the interaction region, and by a translating-slit scanner in the middle of the region. A downstream analyzing magnet separated the Ne^{2+} products from the parent Ne^+ beam. A spherical electrostatic deflector directed the Ne^{2+} products onto a biased stainless-steel plate, from which secondary electrons were detected by a microsphere-plate electron multiplier and counted. The absolute efficiency of the photoion detector (0.210 ± 0.005) was determined by measuring the photoion current with an averaging sub-femtoampere meter and comparing it to the measured count rate. The photon beam was mechanically chopped at 0.5 Hz to separate photoions from Ne^{2+} ions produced by stripping collisions of Ne^+ with residual gas in the ultra-high vacuum system. The photon energy and resolution were selected by a precision curved-grating monochromator. The undulator gap was set to maximize the photon intensity at each selected energy. The photon flux was recorded by a calibrated silicon X-ray photodiode, and was typically $2\text{--}3 \times 10^{13}$ photons/second at an energy of 45 eV and a bandwidth of 22 meV.

The absolute photoionization cross-section measurements taken at an energy resolution of 22 meV are compared in Figure 1 with the results of the *ab initio* Breit-Pauli R-matrix theoretical calculation. Two distinct threshold steps are evident at 40.866 eV and 40.963 eV, corresponding to non-resonant photoionization from the $^2\text{P}_{1/2}$ metastable state and the $^2\text{P}_{3/2}$ ground state, respectively. The calculation represents a sum of the cross sections for photoionization from the ground and metastable states, weighted by their statistical

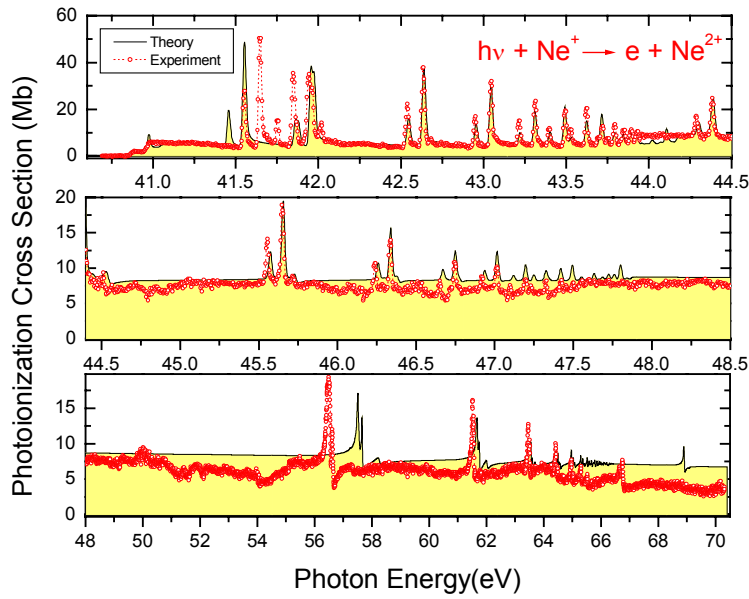


Figure 1. Comparison of absolute measurements (open circles connected by dashed lines) and Breit-Pauli R-matrix theory of McLaughlin (solid curve with shading) for photoionization of Ne^+ . The theory has been convoluted with a Gaussian of 22 meV FWHM to simulate the bandwidth of the experiment.

weights (2/3 and 1/3, respectively). The calculated non-resonant cross section is almost indistinguishable from the absolute measurement in the energy range 41-44 eV, but diverges from the experiment at higher energies. The origin of the broad structures in the measurements above 44 eV may be interleaved series of $2s2p^4(^1S)ns\ ^2S$ window resonances similar to, but broader than, those observed by Caldwell et al [4] in photoionization of fluorine, which is isoelectronic with Ne^+ . It is noteworthy that the predicted energy of the lowest- n resonance differs from experiment by about 100 meV, whereas most of the higher- n resonance energies are in agreement within 10 meV or better. The predicted energy of the $2s2p^5(^3P_2)3p$ resonance feature lies above the measured value of 56.49 eV by more than 1 eV, although the complex lineshapes are similar. A predicted sharp resonance near 69 eV is absent in the experimental data.

A detailed spectroscopic analysis of the resonance structure was performed in order to assign the observed features, which correspond to three Rydberg series of resonances converging to the $2s^22p^4\ ^1D_2$, $2s^22p^4\ ^1S_0$ and $2s2p^5\ ^3P$ excited states of Ne^{2+} at 44.167 eV, 47.875 eV and 66.292 eV, respectively from the ground state of Ne^+ . The measurements along with their assignments are presented in Figure 2. The first two Rydberg series consist of pairs of sharp resonances separated by 97 meV that are distinguishable for autoionizing states with principal quantum numbers n as high as 25. The doubling corresponds to excitation from the ground-state and metastable-state components present in the ion beam. Resonances corresponding to the $2s2p^5(^3P)np$ series are sufficiently broad that components due to excitation from the ground and metastable states of Ne^+ are unresolved, except for the lowest 2p resonance near 42 eV.

Quantum-defect analyses were performed for each of the observed Rydberg series. The lowest members of the $2s^22p^4(^1D_2)nl$ and $2s^22p^4(^1S_0)nl$ Rydberg series were found to exhibit anomalous behavior with respect to their energy positions and relative resonance strengths, making it difficult to assign the features between 41.5 eV and 42.1 eV

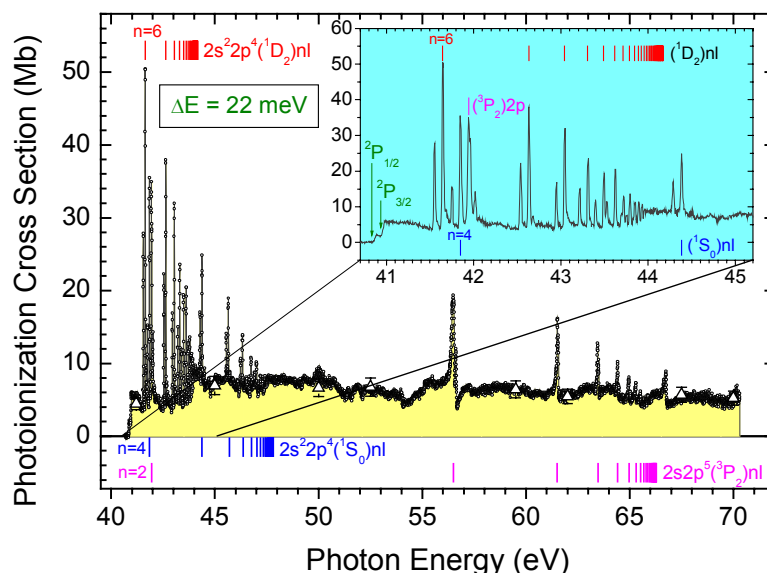


Figure 2. Absolute cross-section measurements for photoionization of Ne^+ (triangles with error bars), to which broad photon energy scan taken at a resolution of 22 meV and a step of 4 meV was normalized. Three Rydberg series of resonances converging to excited states of Ne^{2+} are identified. The inset shows the measurements in the low-energy region on an expanded photon energy scale.

unambiguously. Each series converges to the known spectroscopic limit, independently verifying the photon energy calibration. This apparent breakdown of L-S-J coupling was not observed in photoionization of neutral fluorine [4]. It is surprising that such a dramatic change occurs suddenly along an isoelectronic sequence, motivating follow-up photoionization measurements on other members of this sequence (e.g. Na^{2+}).

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